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Advanced Optimized Quantum Learning for Robust Water Quality Assessment with an IoT Sensor Data

Sakthivel Balu[1*], Sheik Mohammed Abdul Raghabu[1], Ponnrajakumari Mahalingam[2], Jayaram Krishnasamy[3], Jeya Prakash Kadambarajan[4], Deivasigamani Subbramania Pattar[5]

[1] Department of ECE, Pandian Sarswathi Yadava Engineering College, Sivagangai 630561, India
[2] Department of ECE, Velammal Engineering College, Chennai 600066, India
[3] Department of ECE, Kalaignarkarunanidhi Institute of Technology, Coimbatore 641402, India
[4] Department of ECE, Kalasalingam Academy of Research and Education, Virudhunagar 626126, India
[5] FETBE, UCSI University, Kuala Lumpur Campus, Kuala Lumpur 56000, Malaysia

Corresponding Author Email: 786sakthivel@gmail.com

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ABSTRACT

In these decades smart transformation and the digital world are emerging with an effective enhancement. Meanwhile, the management of water quality has also become an important factor in ensuring public health and environmental sustainability. This work presents a real-time water quality prediction by integrating with an Internet of Things (IoT) based sensor data and an optimized quantum convolutional neural network (QCNN) method. The continuous update of water data namely pH, turbidity, dissolved oxygen, and temperature is collected from various sensors fitted inside water bodies. The dataset is gathered by using these sensors that are dynamically monitored using a QCNN method for efficient predictive accuracy and computation. Initially, the important features from the data are extracted using Modified Variational Autoencoder (M-VAE). The QCNN method works on a quantum computing principle that is suitable to handle complex, high-dimensional data. To improve accuracy in higher terms, the QCNN parameters are fine-tuned using a metaheuristic optimization. Therefore, the proposed algorithm of optimized QCNN ensures robustness and reliable performance of water quality in real-time. The validation results of the proposed methodology demonstrate prior deep learning models in terms of classification metrics. Finally, the proposed work satisfies the advancement in real-time water quality prediction and also contributes to a better solution for sustainable water resource management.

1. INTRODUCTION

Water quality has been a critical factor in environmental health and public safety in recent times [1]. The worst water quality harmfully affects ecosystems and also leads to biodiversity loss and aquatic life disruption [2, 3]. Contaminants like heavy metals, pathogens and pesticides can lead to natural habitat degradation which affects both flora and fauna [4]. Also, contaminated water risks the health of humans by causing various diseases namely cholera, dysentery and hepatitis. The World Health Organization (WHO) reports that millions of people suffer from waterborne diseases annually which also highlights the urgent need for effective monitoring and management of water resources [5]. Therefore, preserving high water quality standards is essential to save both ecosystems and human populations from harmful pollutants.

The increase in water pollution and health issues highlights the requirement for proactive water quality prediction [6]. The traditional form of water quality evaluation involves periodic sampling and laboratory analysis which are insufficient for timely detection and response. These techniques are not only time-consuming but also provide limited water conditions pictures and fail to capture dynamic changes. Several prevention methods are used to maintain and improve water quality in the priory. Physical methods include filtration and sedimentation that only remove particulate matter from water [7]. Chemical treatments namely chlorination and ozonation that used to disinfect water to avoid pathogens. Biological techniques are used as biofilters and constructed wetlands that involve natural processes to degrade pollutants.

These traditional methods have many limitations, regular maintenance requirements, the impact of potential environmental and the inability to detect and respond to sudden changes in water quality [8]. Therefore, there is an advanced technology need for real-time water quality management solutions by offering continuous monitoring and early warning. This prediction can prevent health hazards and environmental degradation at an earlier stage. Effective prediction also ensures safer water to consume, agriculture and recreational activities.

For an accurate and reliable prediction, the DL has emerged as a powerful tool of it. The DL method can provide an effective solution even in large datasets and complex patterns. It can identify patterns and correlations significantly than the traditional methods [9]. Some of the popular methods of DL used for real-time prediction are Convolutional Neural Networks (CNNs) are effective for spatial data analysis, Recurrent Neural Networks (RNNs) use time-series data to predict future, Long Short-Term Memory Networks (LSTMs) capture long-term dependencies in sequential data, Autoencoders learns an efficient data representation, Generative Adversarial Networks (GANs) provides a generate realistic synthetic data that suitable to simulate and training predictive models, Graph Neural Networks (GNNs) are Capable to handle a relational data respectively. Each method has a unique style of prediction and various performances based on complexity and data nature [10]. Therefore, accurate and reliable water quality predictions can be attained only by using an appropriate model and optimizing it. Despite their effectiveness, these methods often face challenges when dealing with highly complex, high-dimensional datasets. Additionally, their dependency on large, labeled datasets and susceptibility to overfitting can limit their generalizability and practical utility in certain scenarios.

This paper proposes IoT data with an optimized Quantum Neural Network (QNN) for real-time water quality prediction. The system used a network of IoT sensors that were placed in various water bodies to continuously collect water data such as pH, turbidity, dissolved oxygen and temperature. These sensors are used to transmit real-time cloud data to a processor where an advanced computational method of Quantum Neural Networks (QNNs) is used for prediction. The QNN can explore a vast solution space by identifying optimal patterns and correlations simultaneously. To improve performance further, an optimization model is used to fine-tune the QNN parameters to attain a reliable and optimal solution in water quality predictions. The novelty of the proposed system lies in integrating IoT-based real-time water quality monitoring with an optimized QCNN. It uses quantum principles to handle high-dimensional data and metaheuristic optimization for enhanced predictive accuracy and robustness.

The paper is organised as related work in section 2 which carries a literature work on existing systems, section 3 discusses the material and methods of proposed work that includes the proposed architecture and workflow of it, section 4 explores the result and discussion of the proposed methodology with an existing work comparison and section 5 summarise the work with a conclusion.

2. RELATED WORKS

Existing water quality prediction methods can be broadly categorized based on the type of model and the data source used. From a model perspective, traditional machine learning techniques have been extensively applied. It is focused to on optimizing parameters for improved accuracy. Shams et al. [11] focused on the high accuracy of water quality index identification through various machine learning (ML) models. It uses grid search for optimizing parameters across four classifications and four regression models with result demonstrations.

Xin and Mou [12] identified sulphite, pH, solids, and hardness as critical factors for water quality detection. It highlights the effectiveness of XGBoost, CAT Boost and LGBM models. These models were optimized through cross-validation and hyperparameter tuning that shows robust performance in large-scale water quality detection.

Wang et al. [13] developed an event-triggered fuzzy model to enhance prediction in complex environments. It improves training efficiency by 57.94% for total phosphorus prediction and by 48.31% for biochemical oxygen demand prediction.

Xiang et al. [14] focused on water clarity retrieval in turbid waters that achieves an MAE of 21%-26% and RMSD of 0.3-2.8 meters. The model performed robustly even in extremely turbid waters with MAPE of 22%-25%. Wang et al. [15] worked on a modified iterative soft threshold method that omits the soft threshold to reduce uncertainties. It trains in an unsupervised manner using a loss function with a smooth penalty.

Rivero et al. [16] presented a real-time simulation framework for the effects of spray water on automotive LIDAR sensors that includes other adverse conditions such as dirt, exhaust gases, snow, rain, and fog. Musleh [17] used several ML methods which use a Bagging classifier, Logistic regression, J48, Random Forest and AdaBoost for water potability assessment. The Random Forest, J48 and the Bagging classifier showed high effectiveness.

Regarding data sources, laboratory datasets, as demonstrated by Barroso et al. [18], provide detailed insights into water quality but lack real-time adaptability. They assessed the water quality with 10,000 data of the Manso River reservoir that contains physicochemical parameters, metals, microbiological indicators, biomonitoring, and land use data. Higher concentrations of solids and metals (Fe and Mn) were linked to local geochemistry and mining activities.

Real-time monitoring data from sensors, as highlighted by Mohseni et al. [19], are used to estimate the Weighted Arithmetic Water Quality Index using various machine learning methods. Extreme gradient boosting (XG-Boost) achieves a higher accuracy in predictions with a real-time dataset collected from Ujjain, Madhya Pradesh, India. It showed superior performance with R2=0.96, RMSE=2.169, and MAE=2.013 respectively. Additionally, climate and environmental data provide a broader context for water quality assessment, as demonstrated in the climate-driven models of Aranay et al. [20]. They presented a deep active genetic learning method with combining deep active learning and a genetic model to detect harmful algal blooms in New York using climate data to attain a classification accuracy of 97.14%.

3. MATERIALS AND METHODS

3.1 Materials

The provided diagram Figure 1 presents the proposed system architecture for collecting IoT sensor data to predict water quality using an optimized QCNN model. The system is composed of several components that play a crucial role in the data collection and analysis process.

To attain dynamic water quality, real-time water data is taken by using four types of sensors that are connected to the Arduino controller such as:

- **Temperature Sensor:** Measures the temperature of the water that can affect the chemical and biological processes in the water.
- **pH Sensor:** Determines the acidity or alkalinity of the water which is crucial to assess the suitability of water for various uses. The pH sensor was chosen to measure and monitor water's suitability for various uses, such as drinking, irrigation, and supporting aquatic life.

- **Turbidity Sensor:** Measures the clarity of the water that indicates the presence of suspended particles that might affect water quality. The turbidity sensor was selected because it provides valuable insights into the presence of harmful contaminants that could degrade water quality.
- **Dissolved Oxygen Sensor:** Assesses the amount of oxygen dissolved in the water which is an important parameter for aquatic life and overall water health. The dissolved oxygen sensor was chosen due to its importance in assessing the ecological balance of aquatic environments.

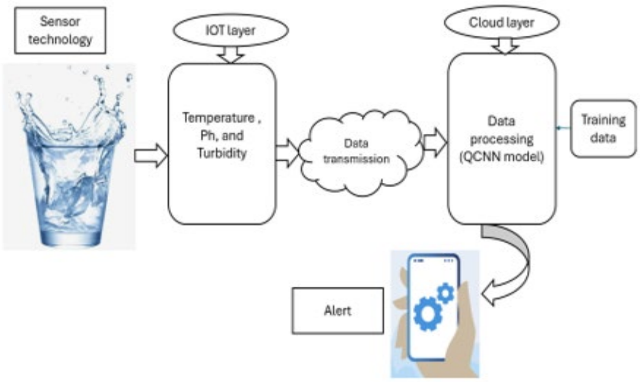


Figure 1. Proposed hardware block

3.2 Arduino controller

It collects data from all the sensors processes this data and serves as the central hub for communication with other system components. It handles data input and process signals to execute control commands based on predefined parameters.

3.3 IoT cloud

The controller-processed data is sent to the IoT cloud. This cloud service stores the data to carry a remote monitoring and further analysis. The IoT cloud acts as a repository where historical data are collected and facilitates the training and evaluation of the optimised QNN model for water quality prediction.

3.4 Proposed optimised QNN methods

3.4.1 M-VAE

A VAE is a probabilistic generative model that learns to encode input data into a latent space and then decode from this latent space to reconstruct the original input. In a Modified VAE, enhancements or adjustments are made to improve the model's performance or adapt it to specific types of data or tasks. The goal of a VAE is to learn a latent space representation of the input data such that the reconstructed data closely resembles the original input. The encoder network maps an input x to a distribution in the latent space. This is typically parameterized as a Gaussian distribution with mean μ and standard deviation σ:

$$q(z|x) = \mathcal{N} * (z; \mu(x), \sigma^2(x)) \tag{1}$$

where, z is the latent variable. To sample from the distribution $q(z|x)$, a reparameterization trick is used:

$$z = \mu(x) + \sigma(x). \epsilon \tag{2}$$

where, ϵ is a random noise vector sampled from a standard normal distribution $\mathcal{N}$ *(0,I)*.The decoder network maps the latent variable z back to the data space, producing a distribution over possible data points:

$$x' = p(x|z) \tag{3}$$

where, x' is the reconstructed data. The VAE is trained to maximize the Evidence Lower Bound (ELBO) on the log-likelihood of the data:

$$L_{\text{ELBO}} = \mathbb{E}_{q(z|x)}[logp(x|z) - KL[q(z|x)\}\}p(z)] \tag{4}$$

where, KL denotes the Kullback-Leibler divergence between the posterior $q(z|x)$ and the prior $p(z)$, often assumed to be a standard normal distribution N(0,I). Expanding this, the ELBO can be written as:

$$L_{\text{ELBO}} = -KL[q(z|x)||p(z)] + \mathbb{E}_{q(z|x)}[logp(x|z)] \tag{5}$$

The hyperparameters of VAE include latent space dimensionality, the rate at which the model learns during training, the number of samples processed before the model's parameters are updated, the number of layers, the number of neurons per layer, and activation functions used in both the encoder and decoder. In modified VAE, these parameters are tuned using a metaheuristic optimizer to achieve higher accuracy in water quality prediction.

Unlike the traditional VAE, M-VAE uses Gaussian distribution in its latent space to capture more complex patterns in the data. The major advantage of using M-VAE for feature extraction is to better handle high-dimensional and complex water quality datasets.

3.4.2 QCNN algorithm

The QCNN method is applied for a data classification which is combined with a CNN model that is given in Figure 2. This method is processed in quantum computing principles to enhance the feature extraction to achieve an efficient classification. The QCNN procedures are explained in the following.

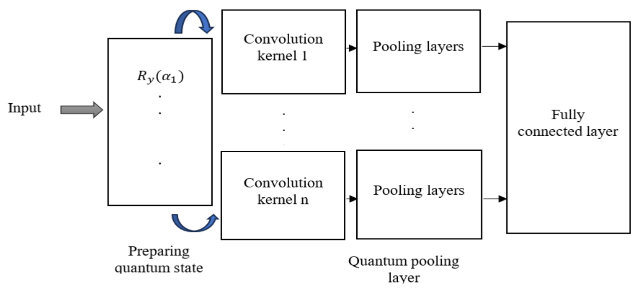


Figure 2. QCNN architecture

Preparing the quantum state

Initially preparing the data for quantum processing is executed. Consider quantum systems with a limited number of qubits available that processed a dimensionality data reduction in qubits. Assume every data sample is an n-dimensional vector and also minimise the dimensionality of the data sample to m dimensions to fit within the quantum system's capacity. Next, the minimised data vector is normalized in range [0,1] as $x = [x1, x2, \dots, xm]$ and then converted into angle information suitable for quantum encoding using $\alpha i = \pi xi$ that resulted as angle vector $\alpha = [\alpha 1, \alpha 2, \ldots, \alpha m]$. By encoding IoT data into a quantum state, angle data (α) to measure angle rotation for quantum gates. Specifically, each α is used as the rotation angle for a Ry gate for every qubit. The Ry gate is a quantum gate that rotates the qubit around the y-axis of the Bloch sphere by the specified angle. Here initial quantum state $|0\rangle$ is transformed into a quantum state that represented as $|\ \phi data\rangle = \otimes_{i=1}^{m} Ry(\alpha i)\ |\ 0\rangle$.

Quantum convolutional layer

This layer applies quantum circuits to the encoded quantum state and acts as a quantum filter to extract features in quantum namely superposition and entanglement. Multiple quantum convolution kernels are applied to the quantum state that is configured with various parameters to capture different patterns and features within the data. The quantum convolutional layer in the QCNN architecture used the principles of quantum mechanics like superposition and entanglement for feature extraction. The quantum convolutional layer applies quantum circuits to the quantum state which allows the model to encode complex features in a more compact and efficient manner. The advantage of quantum convolutional layers lies in their ability to perform simultaneous processing of multiple states which enables them to extract richer and more diverse features from water quality data with fewer parameters than classical models.

Quantum pooling layer

Next, the data moves to quantum pooling which minimises the feature maps obtained from the quantum convolutional layer which summarises the extracted features to maintain significant data. This process manages the system's complexity and prepares the data for further processing. The quantum pooling layer performs a dimensionality reduction operation similar to conventional pooling in CNNs. But, it also uses the concept of quantum parallelism. In this layer, the quantum states obtained from the quantum convolutional layer are processed through quantum pooling circuits. The primary advantage of quantum pooling is its ability to reduce the number of qubits needed. It is also used to hold the essential characteristics of the data.

Measurement and classical processing

Then the conversion of quantum data into classical data is processed. The measurement process collapses the quantum states into classical values and provides a new feature vector which is a captured data extraction of quantum layers.

Fully connected classical layer

Converted data is fed into a fully connected classical layer for a final classification task. It trains the feature vectors by using backpropagation methods to achieve higher efficiency and effectiveness in training methods.

Training with backpropagation

The backpropagation is used to train HCNN by using systems like TensorFlow Quantum that facilitate a quantum circuit's numerical simulation in classic systems and implement a gradient descent in quantum systems. The adjoint differentiation model is employed to compute gradients in the quantum to attain an efficient quantum circuit training model.

To enhance the accuracy of the QCNN method of prediction, the hyperparameter of QCNN is tuned by using a Siberian Tiger Optimization (STO) algorithm [21, 22]. Table 1 lists the parameters of the QCNN method.

These parameters can be tuned using the Siberian Tiger Optimization (STO) algorithm to find the optimal configuration for the QCNN.

Table 1. QCNN hyperparameters

Parameter	Range/Options
Number of Qubits (N)	4 to 16
Quantum Circuit Depth	1 to 10 layers
Types of Quantum Gates	RyR_yRy, RzR_zRz, Hadamard, CNOT, Controlled-Z
Rotation Angles	0 to π\π
Quantum Convolution Kernels	Variable, depending on the design
Quantum Pooling Strategy	Fixed or adaptive strategies
Learning Rate	0.001 to 0.1
Batch Size	16, 32, 64, 128
Number of Epochs	10 to 100
Optimizer	Adam, SGD, RMSprop
Dropout Rate	0 to 0.5

3.4.3 STO method for QCNN parameter tuning

It is motivated using Siberian tigers' characteristics that involve hunting prey and fighting brown bears. Compared to other metaheuristic optimization algorithms, the STO has a faster convergence rate and can easily escape local minima. The mathematical evaluation of these behaviours with an iterative optimization to identify an optimal result for complex issues. This method can effectively fine-tune the parameters of a QCNN to classify the data.

Initialization

Initially, the population of candidate solutions is initialised that represents a set of hyperparameters for the QCNN.

1. **Population Matrix (X)**: Initialize the tiger's positions randomly that represent a candidate solution in each space.
2. **Best Solution (X_best)**: identify the best solution of an objective function value.

Phase 1: Prey Hunting

This phase explores the hunting behaviour of tigers in search space extensively. It selects a prey position with a better objective function value and simulates an attack, resulting in significant changes in its position.

1. **Position Update**:

$$x_{i,j}^{P1s1} = x_{i,j} + rand\left(M_{i,j} - I_{i,j} x_{i,j}\right) \tag{6}$$

where, rand is a parameter that varies from zero to one, $M_{i,j}$ is a member, j is the dimension and $I_{i,j}$ are coefficient varies from zero to two.

2. **Final Position Update**:

$$x_{i,j}^{P1s2} = x_{i,j} + \frac{rand\left(ul_j - ll_j\right)}{t} \tag{7}$$

where, t is the iteration number, and ul and ll denote the lower and upper limits for optimization.

Phase 2: Fighting with a Bear

This phase simulates tigers fighting brown bears. Tigers select a bear position and calculate a new position based on the bear's position. It can be expressed as follows:

1. **Position Update**:

$$x_{i,j}^{P2s1} = \begin{cases} x_{i,j} + rand\left(x_{k,j} - I x_{i,j}\right), F_k < F_i \\ x_{i,j} + rand\left(x_{i,j} - x_{k,j}\right), ELSE \end{cases} \tag{8}$$

2. **Final Position Update**:

$$x_{i,j}^{P2s2} = x_{i,j} + \frac{rand(\,ul_j \;- ll_j\,)}{t} \quad (9)$$

Iterative Process

The STO algorithm iteratively processes these stages to reach an optimal solution. The objective function is set as a function of the accuracy or error rate of the model. The pseudocode of the proposed optimization is given below:

Pseudocode of optimised QCNN

1. Sets the hyperparameters of the QCNN model based on the provided candidate solution.
2. Train specified hyperparameters.
3. Evaluate the trained model on a validation dataset and calculate the accuracy.
4. Represents the accuracy of the trained model on the validation dataset.
5. Returns the validation accuracy as an objective value to maximize during optimization.
6. Randomly initialize the population of candidate solutions.
7. Select candidate solutions based on their fitness scores.
8. Select a prey position for the tiger.
9. Update the tiger's position in the first stage.
10. Finalize the tiger's position update.
11. Select a bear position for the tiger.
12. Update the tiger's position in the first stage of the bear fight.
13. Finalize the tiger's position update during the bear fight.
14. Output the best solution and its accuracy.

By using an optimized QCNN model, the system provided an efficient water quality prediction with advanced quantum computing even in complex water quality data. It also carried reliable and more accurate prediction outcomes. The same iterative steps were followed to tune the hyperparameters of VAE.

3.5 Display alert

The predicted quality data outcomes are transmitted to the IoT cloud where the controller is also linked to a display alert system. This component provides real-time alerts and notifications in the system to ensure immediate awareness of any important changes or issues in water quality parameters. The alerts help in prompt decision-making and corrective actions.

Therefore, overall, an integrated system continuously monitors the quality of water with an integration of IoT technology and predictive analysis using an optimised QCNN model. Thus, the proposed optimised QCNN model is effectively trained with the historical IoT data and optimized to accurately predict future water quality. This method helps to ensure water safety to provide a quality environment.

4. RESULTS AND DISCUSSIONS

The performance of the optimized QCNN model is evaluated and discussed in this section. It handles the IoT sensor data as a dataset and validates an accurate and efficient prediction. It analyses an intricate pattern within water quality datasets and converts in quantum computing principles to extract data from sensors. Also, evaluation of classification metrics like accuracy, specificity, recall, precision, F1 score, and confusion matrix shows its effectiveness.

In Table 2, which compares various techniques for water quality prediction, the proposed "Optimised QCNN" method distinguishes itself by achieving notably high values across different classification metrics. The results are graphically shown in Figure 3.

Table 2. Metrics comparison of proposed and existing methods

Techniques	Specificity (%)	Precision (%)	Recall (%)	F1 Score (%)	Accuracy (%)
Optimised QCNN	98.76	98.15	97.32	98.52	98.55
Graph Neural Networks (GNN) [23]	94.85	95.26	95.12	96.29	95.11
Generative Adversarial Network [24] (GAN)	93.1	94.73	93.84	95.65	94.65
Long short-term memory (LSTM) [25]	91.28	92.53	92.29	93.26	93.82
Recurrent Neural Network (RNN) [26]	89.37	90.86	90.18	91.46	92.15
CNN [27]	88.24	88.43	89.23	90.34	89.32

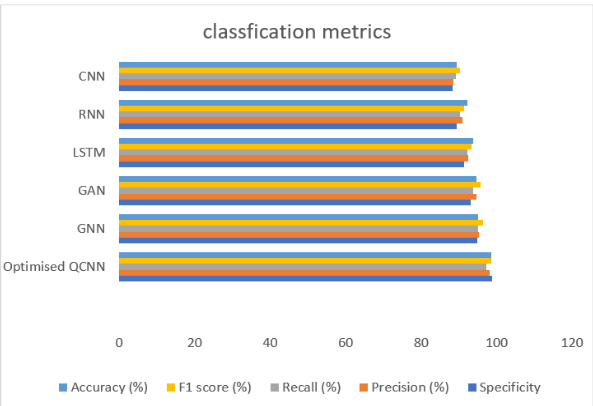
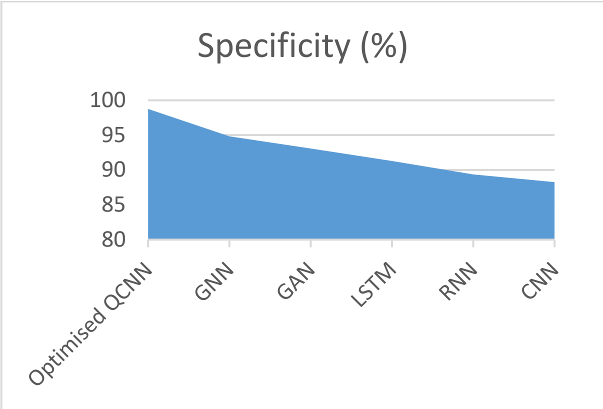


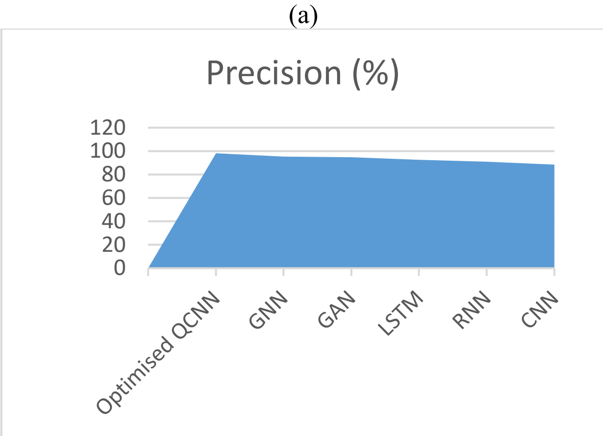
Figure 3. Performance metrics for proposed and prior methods

The proposed mode achieved higher values in all the metrics among all other works whereas a high specificity of 98.76% is attained that correctly identifies negative instances with a minimal rate of false positives. Also, a precision score of 98.15% is achieved which recognises positive instances with higher reliability of water quality anomalies. The proposed recall of 97.32% attained effectiveness in capturing true positive instances to detect potential contaminants or water quality deviations. The impressive F1 score of 98.52% shows its robustness in handling various water quality prediction tasks. Lastly, it achieves an Accuracy of 98.55% which presents superiority in water prediction. The results are graphically shown in Figure 4.

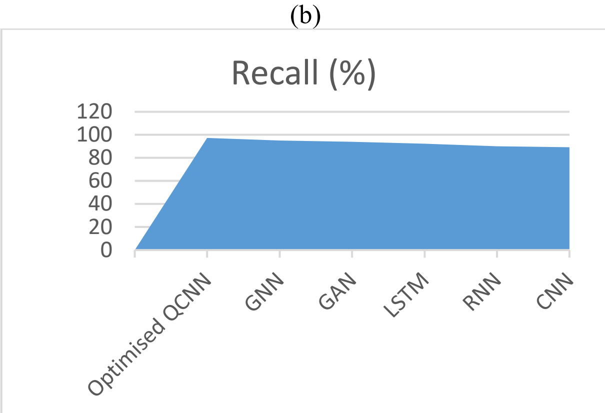
For the fair comparison of the Optimized QCNN model, its performance on individual water quality parameter prediction tasks, such as pH, turbidity, and dissolved oxygen (DO) are analyzed. This analysis demonstrates the versatility of the model in handling different water quality metrics critical for environmental monitoring. The results are given in Table 3.



(a)



(b)



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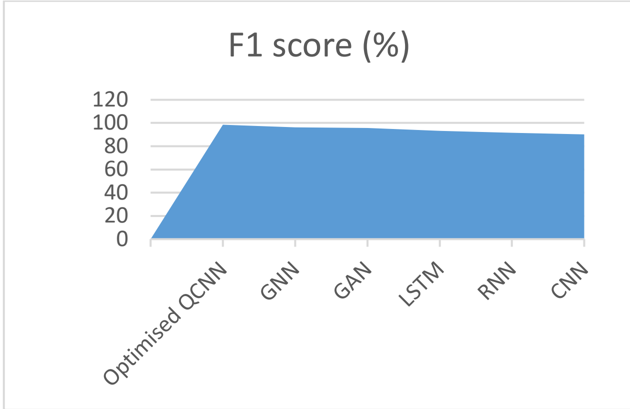
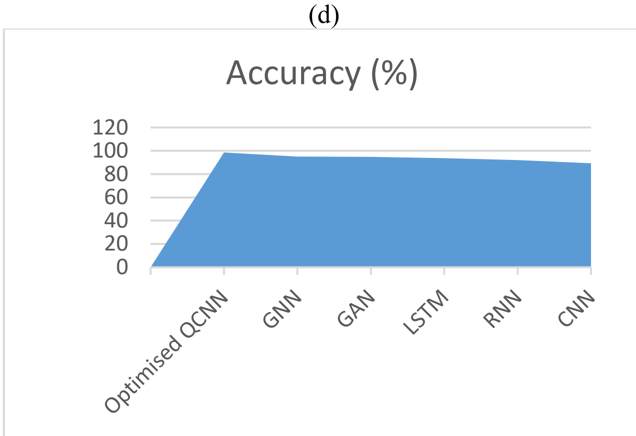


(d)



(e)

Figure 4. (a) Specificity metrics, (b) precision metrics, (c) recall metrics, (d) F1 score metrics and (e) accuracy metrics

The model consistently achieved high specificity and assures accurate identification of negative instances such as when water quality deviations are absent. To address the recommendation, an error analysis is conducted to identify potential prediction biases in the optimized QCNN model. The data quality issues like noisy or incomplete IoT sensor data affect the performance, especially for parameters like turbidity. Additionally, the model's structure struggled to capture dynamic temporal dependencies in rapidly fluctuating parameters like dissolved oxygen. The dataset imbalance also contributed to minor recall deviations.

Table 3. Metrics comparison of different quality metrics

Parameter	Specificity (%)	Precision (%)	Recall (%)	F1 Score (%)	Accuracy (%)
pH	97.85	97.42	96.98	97.20	97.36
Turbidity	98.12	97.89	97.56	97.72	97.95
Dissolved Oxygen (DO)	98.67	98.41	97.93	98.16	98.35

5. CONCLUSION

In this water quality prediction, the proposed work presents sensor data that is processed with predictive analytics from IoT devices. It proposed an optimized QCNN for an efficient and qualitative prediction to achieve its effectiveness. The IoT sensor data integrated with an optimized QCNN technique demonstrates its intricate patterns of water quality datasets. The experimental result of optimized QCNN proves efficiency with classification metrics. With specificity at 98.76%, the model identifies negative instances to ensure minimal false positives and bolster water safety protocols. Furthermore, precision achieves 98.15% in detecting positive instances which is essential for contaminants or deviations. The QCNN's recall score of 97.32% shows its effectiveness in capturing true positive instances for quality management. Meanwhile, this work has a higher accuracy of 98.55% and an effective balancing F1 score of 98.52% respectively**.** Therefore, this optimized QCNN model holds an accurate and timely prediction of water quality than the prior methods. Through its integration into the IoT system, this optimized QCNN method provides a transformative model shift in water quality prediction for more efficient and proactive management of water systems. To enhance the applicability of the Optimized QCNN model, future work should focus on extending its implementation to different water bodies, such as lakes and oceans which shows varying environmental conditions and water quality patterns. Additionally, the model can be adapted to predict more complex water quality parameters including heavy metals and organic pollutants, which are critical for comprehensive water quality assessment.

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